2-2012

Heterogeneous Multiscale Modeling of Advection-Diffusion Problems

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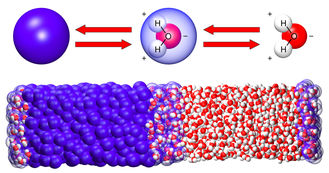
Introduction

Many problems in science and engineering involve multiple spatial and temporal scales differing by several orders of magnitude. Traditionally, the mathematical models for studying these problems fit into two categories: continuum-level and atomistic-scale.

Continuum-level models, derived from conservation laws, typically treat physical systems at a macroscopic scale. Information at the atomistic-scale is incorporated through simplifying assumptions about the physical system to obtain constitutive equations. Generally this approach works well, allowing for efficient numerical simulation of large systems. However, it is not always possible to derive the necessary constitutive relations to accurately describe the relevant physical processes. Problems modeled purely at the atomistic-scale retain detail lost in continuum approaches allowing for highly-predictive simulations. Unfortunately, the computational requirements to track all the atoms in a system greatly limits simulation size.

Multiscale modeling strives to combine these two approaches balancing the efficiency of a continuum model with detailed atomistic-scale information. In this work, we investigate the application of the heterogeneous multiscale method (HMM) to advection-diffusion problems where unknown transport coefficients are supplied by Brownian motion simulations. Specifically, we present our new multiscale modeling simulation framework, and address questions regarding how simulation parameters in the microscale model affect the precision of the macroscopic transport coefficients.



Heterogeneous Multiscale Method

The Heterogeneous Multiscale Method [2,3,4] is a top down general template for constructing multiscale methods to solve problems with unclosed macroscopic models.

The specific macro/micro models, how to link the models, and how to compute the data for the macroscale are not prescribed by HMM but rather chosen to fit the particular application creating.

Thus there are four key decisions when constructing a HMM based model:

- What is the appropriate macroscale solver?
- What microscale model will produce the desired data?
- How to make the microscale consistent with the macroscale state?
- How to estimate macroscale data from the microscale results?

With these choices made, the simulation proceeds as follows:

- Initialize microscale model from macro data
- Run microscale solver until local relaxation
- Estimate macro data from microscale results
- Advance macroscale solver
- Repeat

Macro Model

The macroscale model is the standard advection-diffusion equation,

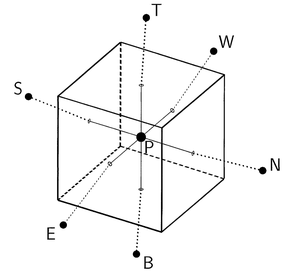
$$\partial_t u + \nabla \cdot (\boldsymbol{\beta} u) - \nabla \cdot (D \nabla u) = f$$

where

- u - density
- $\boldsymbol{\beta}$ - advection coefficients
- D - diffusion coefficients
- f - external forcing

We suppose the transport coefficients are unknown and must be supplied by the microscale model.

The equation is discretized in space using finite volumes with u values at cell centers and the transport coefficients at cell faces.



The system integrated in time using the method of lines approach with standard ODE solvers:

- Explicit Runge-Kutta, Diagonally Implicit Runge-Kutta (DIRK), Singly Diagonally Implicit Runge-Kutta (SDIRK), or Additive Runge-Kutta

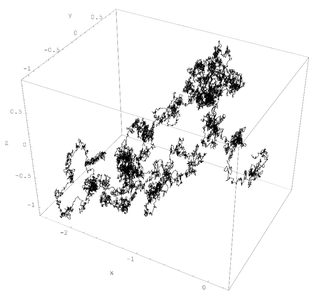
Micro Model

The microscale is modeled as Brownian motion which consists of Newton's second law with drag due to the surrounding fluid and a random force from impacts with molecules in the surrounding fluid.

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i \ , \qquad \frac{d\mathbf{v}_i}{dt} = -\gamma \mathbf{v}_i + \sqrt{2S}\boldsymbol{\xi}_i$$

where

- $\mathbf{x}_i$ - i^{th} particle position
- $\mathbf{v}_i$ - i^{th} particle velocity
- $\sqrt{2S}$ - scaling factor determined by properties of surrounding fluid
- γ - coefficient of friction
- $\boldsymbol{\xi}_i$ - Gaussian white noise



Simulations are carried out at each finite volume face and advanced in time using a variety of ODE methods. Evaluating the microscale model is the dominant computational cost of the multiscale method.

Coupling the Models

For consistency with the local macroscale state, each microscale simulation is initialized using the average density at the face and the simulation temperature.

The model is run to time $t_f = t_r + m\Delta t$ where t_r is the relaxation time of the system approximately $1/\gamma$ [5].

Advection and diffusion coefficients are obtained by tracking particle positions from t_R to t_f and computing the first and second sample moments of particle displacements [1,5].

$$\beta_i = \frac{1}{t}\langle \Delta \mathbf{x}_i(t_f) \rangle \ , \qquad D_i = \frac{1}{2t}\langle \Delta \mathbf{x}_i^2(t_f) \rangle$$

where

$$\langle \Delta \mathbf{x}_i^k(t_f) \rangle = \frac{1}{m}\sum_{j=1}^{m} \left[\mathbf{x}_i(j\Delta t) - \mathbf{x}_i((j-1)\Delta t) \right]^k$$

These results are then averaged over all N particles,

$$\beta = \frac{1}{N}\sum_{i=1}^{N} \beta_i \ , \qquad D = \frac{1}{N}\sum_{i=1}^{N} D_i$$

Questions

- How does N affect the quality of transport coefficients?
- How large should t_f be to obtain accurate statistics?
- How does the choice of microscale stepper affect convergence?
- How does the choice of macroscale time stepper affect overall accuracy?
- How can the number of calls to the microscale simulation be minimized?

Future Work

Ultimately, the goal of this work is to develop models for multiscale and multiphysics problems such as fusion plasma simulation.

Continuum approaches, which are variations of magnetohydrodynamics (MHD), attempt to more accurately resolve the interactions of electrons and ions across drastically different scales.

Applying the HMM to such a new context will provide new tools for understanding complex problems as well as extending the breadth of HMM applicability.

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